

1.0165415.7

Page 1

*Yerulov*  
14/11/04  
*Yerulov*  
1624

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=> file reg  
COST IN U.S. DOLLARS  
SINCE FILE ENTRY TOTAL  
SESSION  
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 08:30:26 ON 10 DEC 2004  
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STRUCTURE FILE UPDATES: 8 DEC 2004 HIGHEST RN 795251-52-4  
DICTIONARY FILE UPDATES: 8 DEC 2004 HIGHEST RN 795251-52-4

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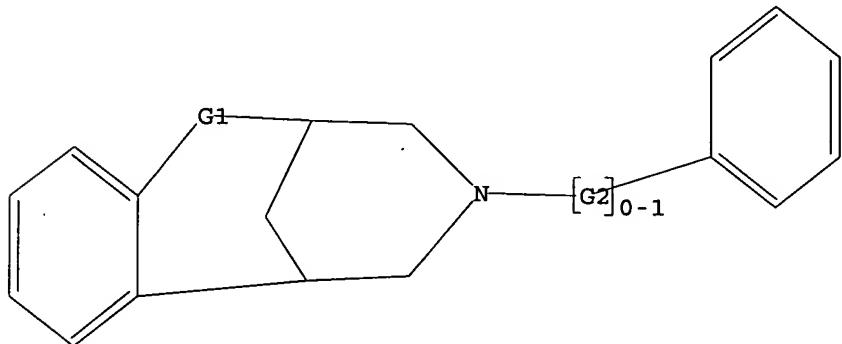
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10764167.str

L1 STRUCTURE UPLOADED

=> d 11  
L1 HAS NO ANSWERS  
L1 STR



G1 CH2,CF2  
G2 H,Me,CH2,Et,n-Pr,n-Bu

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss full  
FULL SEARCH INITIATED 08:30:54 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 578205 TO ITERATE  
  
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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.03  
  
FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 578205 TO 578205  
PROJECTED ANSWERS: 27 TO 57

L2 27 SEA SSS FUL L1

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COST IN U.S. DOLLARS	ENTRY	SESSION
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FILE COVERS 1907 - 10 Dec 2004 VOL 141 ISS 25  
 FILE LAST UPDATED: 9 Dec 2004 (20041209/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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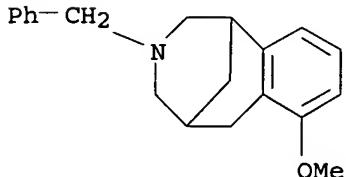
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 DN 138:348736  
 TI Nicotinic acetylcholine receptor agonists in the treatment of restless legs syndrome  
 IN Saltarelli, Mario David  
 PA Pfizer Products Inc., USA  
 SO PCT Int. Appl., 37 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

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PI WO 2003037329	A1	20030508	WO 2002-IB4379	20021021
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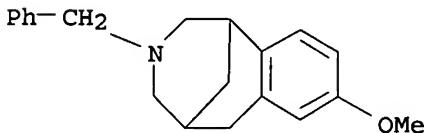
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OS MARPAT 138:348736  
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 248275-97-0 248275-99-2 248276-26-8  
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 519165-35-6 519165-36-7  
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 (Biological study); USES (Uses)  
 (nicotinic agonists for treatment of restless legs syndrome)

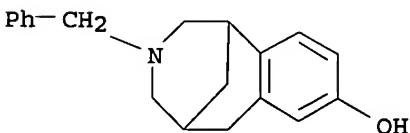
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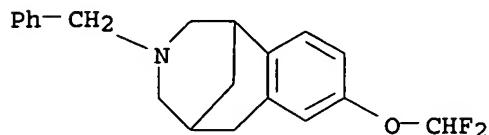


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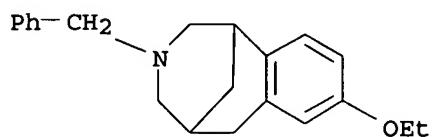
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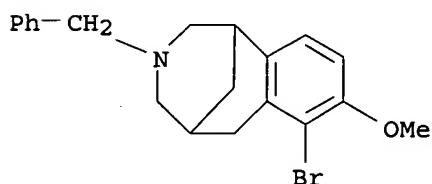
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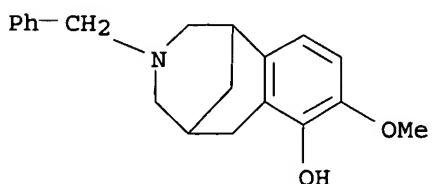
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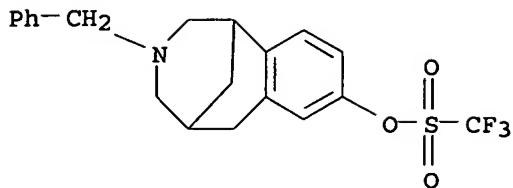
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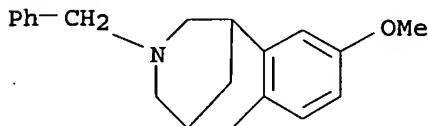


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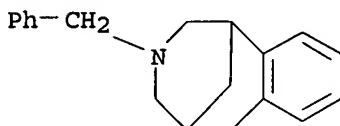
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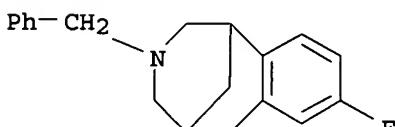
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RN 519165-36-7 CAPLUS  
 CN 1,5-Methano-3-benzazocine, 8-fluoro-1,2,3,4,5,6-hexahydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



AB The invention discloses the use of nicotinic acetylcholine receptor agonists for the treatment of restless legs syndrome (RLS). The invention further discloses the use of a nicotinic acetylcholine receptor agonist in the manufacture of a medicament for the treatment of RLS. The invention also discloses a pharmaceutical composition for the treatment of RLS containing a nicotinic acetylcholine receptor agonist.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1999:708745 CAPLUS  
 DN 131:322551  
 TI Aryl-fused azapolycyclic compounds as nicotine binding inhibitors  
 IN Coe, Jotham Wadsworth

PA Pfizer Products Inc., USA  
 SO PCT Int. Appl., 80 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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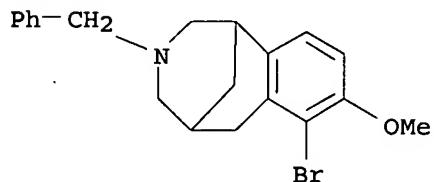
OS MARPAT 131:322551

IT 248276-26-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(Br/OH exchange; preparation of aryl-fused azapolycyclic compds. as inhibitors of nicotine binding to specific receptor sites)

RN 248276-26-8 CAPLUS

CN 1,5-Methano-3-benzazocine, 7-bromo-1,2,3,4,5,6-hexahydro-8-methoxy-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

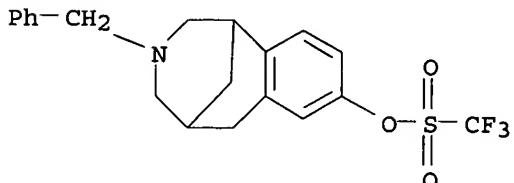


IT 248276-30-4P

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(coupling reactions; preparation of aryl-fused azapolycyclic compds. as inhibitors of nicotine binding to specific receptor sites)

RN 248276-30-4 CAPLUS

CN Methanesulfonic acid, trifluoro-, 1,2,3,4,5,6-hexahydro-3-(phenylmethyl)-1,5-methano-3-benzazocin-8-yl ester (9CI) (CA INDEX NAME)

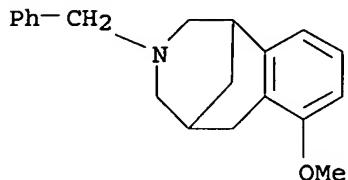


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 248276-36-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (debenzylation; preparation of aryl-fused azapolycyclic compds. as inhibitors of nicotine binding to specific receptor sites)

RN 248275-78-7 CAPLUS

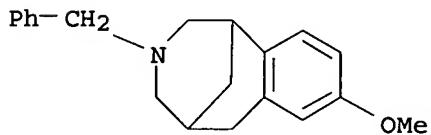
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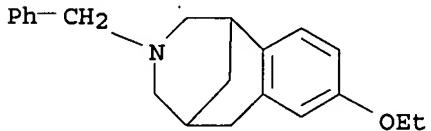
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● HCl

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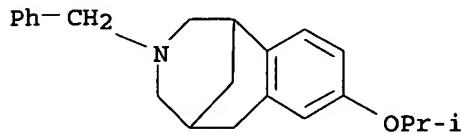
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● HCl

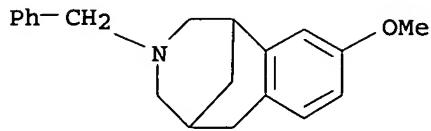
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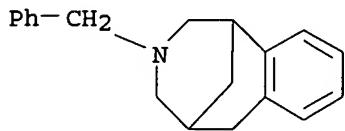
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● HCl

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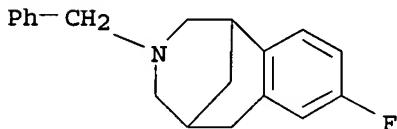
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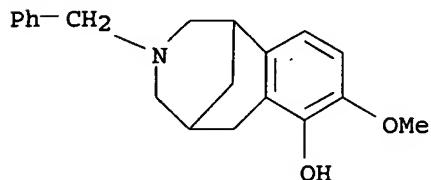
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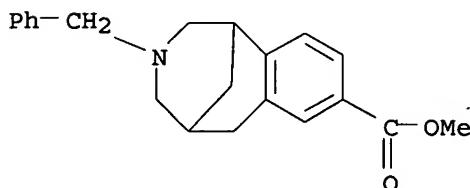
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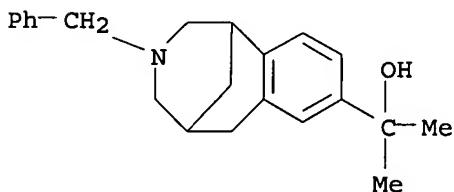


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RN 248276-36-0 CAPLUS

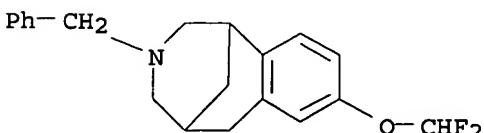
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IT 248275-97-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (demethylation; preparation of aryl-fused azapolycyclic compds. as inhibitors of nicotine binding to specific receptor sites)

RN 248275-97-0 CAPLUS

CN 1,5-Methano-3-benzazocine, 8-(difluoromethoxy)-1,2,3,4,5,6-hexahydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

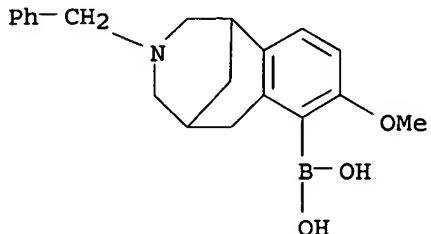


IT 248276-27-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (oxidation; preparation of aryl-fused azapolycyclic compds. as inhibitors of nicotine binding to specific receptor sites)

RN 248276-27-9 CAPLUS

CN Boronic acid, [1,2,3,4,5,6-hexahydro-8-methoxy-3-(phenylmethyl)-1,5-methano-3-benzazocin-7-yl] - (9CI) (CA INDEX NAME)

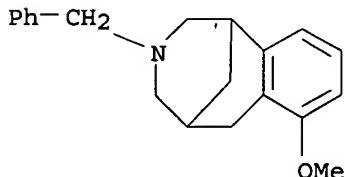


IT 248275-77-6P 248275-93-6P 248275-99-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of aryl-fused azapolycyclic compds. as inhibitors of nicotine binding to specific receptor sites)

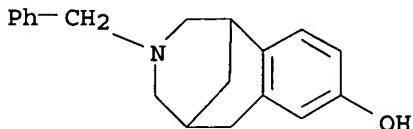
RN 248275-77-6 CAPLUS

CN 1,5-Methano-3-benzazocine, 1,2,3,4,5,6-hexahydro-7-methoxy-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 248275-93-6 CAPLUS

CN 1,5-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-3-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

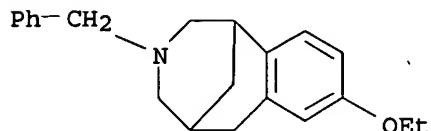


● HCl

RN 248275-99-2 CAPLUS

CN 1,5-Methano-3-benzazocine, 8-ethoxy-1,2,3,4,5,6-hexahydro-3-(phenylmethyl)-

(9CI) (CA INDEX NAME)

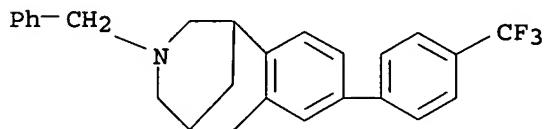


IT 248276-31-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of aryl-fused azapoly cyclic compds. as inhibitors of nicotine binding to specific receptor sites)

RN 248276-31-5 CAPLUS

CN 1,5-Methano-3-benzazocine, 1,2,3,4,5,6-hexahydro-3-(phenylmethyl)-8-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

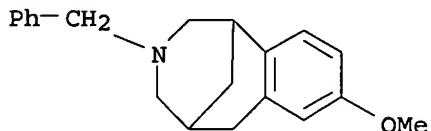


IT 248275-90-3P 248275-92-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (reactions; preparation of aryl-fused azapoly cyclic compds. as inhibitors of nicotine binding to specific receptor sites)

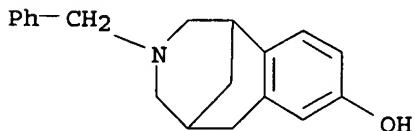
RN 248275-90-3 CAPLUS

CN 1,5-Methano-3-benzazocine, 1,2,3,4,5,6-hexahydro-8-methoxy-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

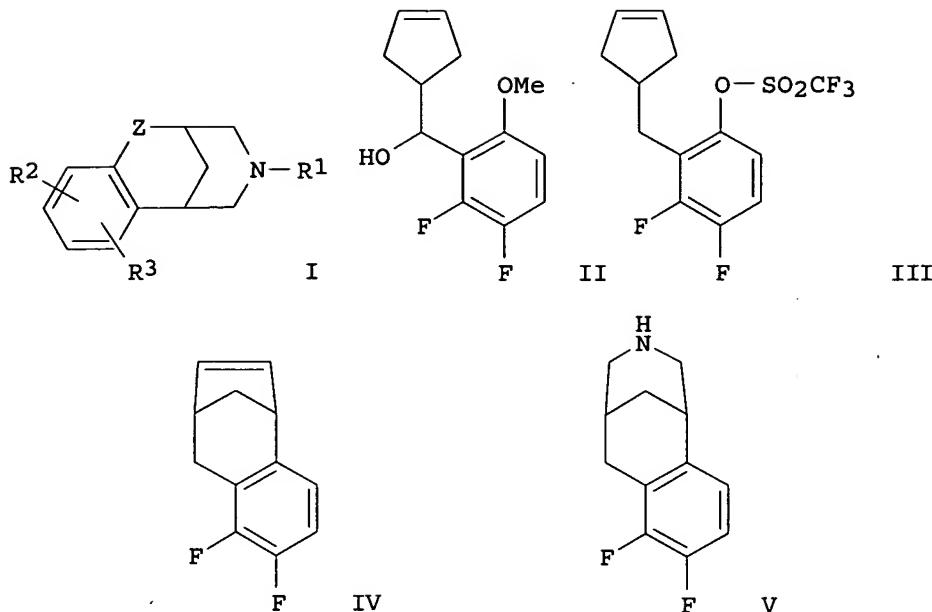


RN 248275-92-5 CAPLUS

CN 1,5-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



GI



AB Compds. of formula (I) and their pharmaceutically acceptable salts, wherein: Z = CH<sub>2</sub>, CO, CF<sub>2</sub>; R<sub>1</sub> = e.g., H, C<sub>1</sub>-6-alkyl, unconjugated C<sub>3</sub>-6-alkenyl, benzyl; R<sub>2</sub>, R<sub>3</sub> are independently, e.g., H, C<sub>2</sub>-6-alkenyl, C<sub>2</sub>-6-alkynyl, hydroxy, nitro, amino, halo, cyano, were prepared as nicotine binding inhibitors (IC<sub>50</sub> < 10 $\mu$ M). Thus, e.g., metalation/addition reaction of 1,2-difluoro-4-methoxybenzene with cyclopent-3-enecarboxaldehyde afforded the methanol II; reduction, demethylation, and sulfonylation afforded triflate III; Heck cyclization to IV was followed by osmylation/oxidation to the diol; the latter was converted to title compound V via oxidative cleavage/reductive amination.

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

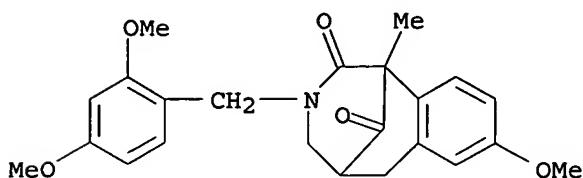
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1997:528299 CAPLUS  
DN 127:109166  
TI Synthesis of a New Tyrosine Analog Having  $\chi_1$  and  $\chi_2$  Angles Constrained to Values Observed for an SH2 Domain-Bound Phosphotyrosyl Residue  
AU Ye, Bin; Yao, Zhu-Jun; Burke, Terrence R., Jr.  
CS Laboratory of Medicinal Chemistry Division of Basic Sciences National Cancer Institute, National Institutes of Health, Bethesda, MD, 20892, USA  
SO Journal of Organic Chemistry (1997), 62(16), 5428-5431  
CODEN: JOCEAH; ISSN: 0022-3263  
PB American Chemical Society  
DT Journal  
LA English  
OS CASREACT 127:109166  
IT 192212-94-5P 192212-95-6P 192212-96-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of constrained tyrosine analog with  $\chi_1$  and  $\chi_2$  values close to SH2 domain-bound phosphotyrosyl residues)

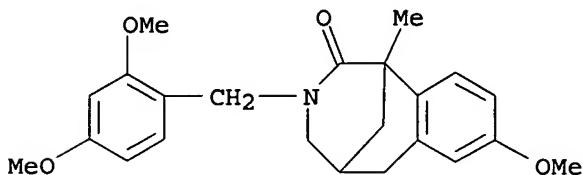
RN 192212-94-5 CAPLUS

CN 1,5-Methano-3-benzazocine-2,11(1H)-dione, 3-[(2,4-dimethoxyphenyl)methyl]-3,4,5,6-tetrahydro-8-methoxy-1-methyl- (9CI) (CA INDEX NAME)



RN 192212-95-6 CAPLUS

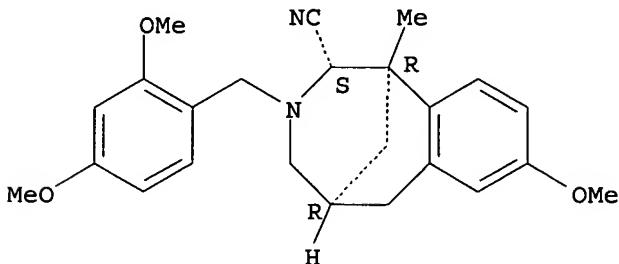
CN 1,5-Methano-3-benzazocin-2(1H)-one, 3-[(2,4-dimethoxyphenyl)methyl]-3,4,5,6-tetrahydro-8-methoxy-1-methyl- (9CI) (CA INDEX NAME)



RN 192212-96-7 CAPLUS

CN 1,5-Methano-3-benzazocine-2-carbonitrile, 3-[(2,4-dimethoxyphenyl)methyl]-1,2,3,4,5,6-hexahydro-8-methoxy-1-methyl-, (1 $\alpha$ ,2 $\alpha$ ,5 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 192212-97-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of constrained tyrosine analog with  $\chi_1$  and  $\chi_2$  values close to SH2 domain-bound phosphotyrosyl residues)

RN 192212-97-8 CAPLUS

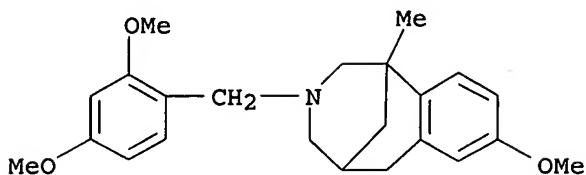
CN 1,5-Methano-3-benzazocine, 3-[(2,4-dimethoxyphenyl)methyl]-1,2,3,4,5,6-hexahydro-8-methoxy-1-methyl- (9CI) (CA INDEX NAME)

10764167

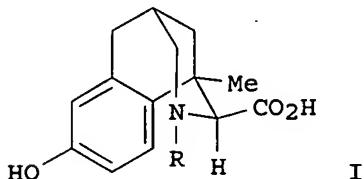
10169415.7

Page 16

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12/11/04  
1624



GI



AB Synthesis is reported of new tricyclic amino acid I ( $R = H$ ), which contains within its structure the elements of a tyrosine moiety having  $\chi_1$  and  $\chi_2$  angles ( $168^\circ$  and  $-95^\circ$ , resp.) constrained to values observed for a phosphotyrosyl (pTyr) residue bound to the 56lck SH2 domain ( $\chi_1$  and  $\chi_2$  values of  $163^\circ$  and  $-94^\circ$ , resp.). Addnl., the  $\phi$  angle of I ( $R = \text{acyl}$ ) correlates well with the  $\phi$  angle of the SH2 domain-bound pTyr residue. I ( $R = H$ ) represents a unique, highly constrained amino acid which may be of value in signal transduction studies.